

We claim:

1. A monocyclopentadienyl complex comprising the structural feature of the formula Cp-Y_mM^A (I), where the variables have the following meanings:

5

Cp is a cyclopentadienyl system having an aryl substituent,

Y is a substituent which is bound to Cp and contains at least one uncharged donor containing at least one atom of group 15 or 16 of the Periodic Table,

10

M^A is titanium, zirconium, hafnium, vanadium, niobium, tantalum, chromium, molybdenum or tungsten or an element of group 3 of the Periodic Table and the lanthanides and

15 m is 1, 2 or 3.

15

2. A monocyclopentadienyl complex as claimed in claim 1 having the formula Cp-Y_mM^AX^A_n (V), where the variables have the following meanings:

20

Cp is a cyclopentadienyl system having an aryl substituent,

Y is a substituent which is bound to Cp and contains at least one uncharged donor containing at least one atom of group 15 or 16 of the Periodic Table,

25

M^A is titanium, zirconium, hafnium, vanadium, niobium, tantalum, chromium, molybdenum or tungsten or an element of group 3 of the Periodic Table and the lanthanides and

m is 1, 2 or 3,

30

X^A the radicals X^A are each, independently of one another, fluorine, chlorine, bromine, iodine, hydrogen, C₁-C₁₀-alkyl, C₂-C₁₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having 1-10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part, NR^{23A}R^{24A}, OR^{23A}, SR^{23A}, SO₃R^{23A}, OC(O)R^{23A}, CN, SCN, β-diketonate, CO, BF₄⁻, PF₆⁻ or bulky noncoordinating anions or two radicals X^A form a substituted or unsubstituted diene ligand, in particular a 1,3-diene ligand, and the radicals X^A may be joined to one another,

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R^{23A}-R^{24A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part, SiR^{25A}₃, where the organic radicals R^{23A}-R^{24A} may also

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be substituted by halogens or nitrogen- and oxygen-containing groups and two radicals R^{23A} - R^{24A} may also be joined to form a five- or six-membered ring,

5 R^{25A} the radicals R^{25A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two radicals R^{25A} may also be joined to form a five- or six-membered ring and

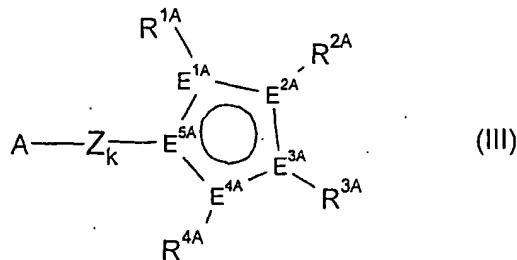
10 n is 1, 2, or 3.

15 3. A monocyclopentadienyl complex as claimed in claim 1 or 2 in which Y is formed by the group -Z_k-A- and together with the cyclopentadienyl system Cp and M^A forms a monocyclopentadienyl complex comprising the structural element of the formula Cp-Z_k-A-M^A (II), where the variables have the following meanings:

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Cp-Z_k-A

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Where the variables have the following meanings:

E^{1A} - E^{5A} are each carbon or not more than one E^{1A} to E^{5A} is phosphorus,

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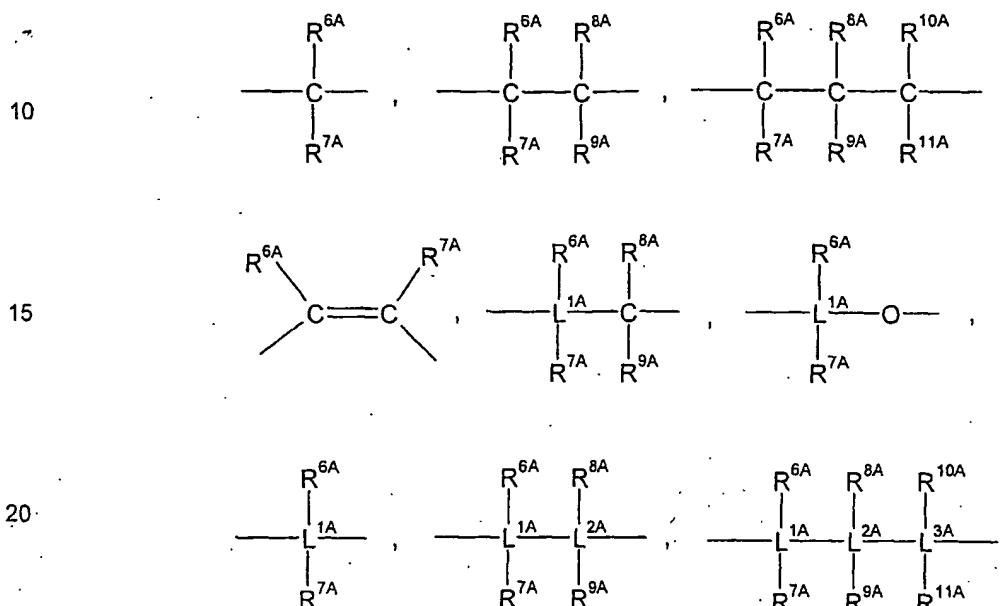
R^{1A} - R^{4A} are each, independently of one another, hydrogen, C₁-C₂₂-alkyl, C₂-C₂₂-alkenyl, C₆-C₂₂-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl radical and 6-20 carbon atoms in the aryl radical, NR^{5A}₂, N(SiR^{5A}₃)₂, OR^{5A}, OSiR^{5A}₃, SiR^{5A}₃, BR^{5A}₂, where the organic radicals R^{1A} - R^{4A} may also be substituted by halogens and two vicinal radicals R^{1A} - R^{4A} may also be joined to form a five-, six- or seven-membered ring, and/or two vicinal radicals R^{1A} - R^{4A} are joined to form a five-, six- or seven-membered heterocycle which contains at least one atom from the group consisting of N, P, O or S and at least one R^{1A} - R^{4A} is a C₆-C₂₂-aryl, where the aryl may also be substituted by N-, P-, O- or S-containing substituents, C₁-C₂₂-alkyl, C₂-C₂₂-alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms,

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R^{5A} the radicals R^{5A} are each, independently of one another, hydrogen, C_1 - C_{20} -alkyl, C_2 - C_{20} -alkenyl, C_6 - C_{20} -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals R^{5A} may also be joined to form a five- or six-membered ring,

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Z is a divalent bridge between A and Cp selected from the group consisting of



$-BR^{6A}-$, $-BNR^{6A}R^{7A}-$, $-AIR^{6A}-$, $-Sn-$, $-O-$, $-S-$, $-SO-$, $-SO_2-$, $-NR^{6A}-$, $-CO-$,
25 $-PR^{6A}-$ or $-P(O)R^{6A}$,

where

$L^{1A}-L^{3A}$ are each, independently of one another, silicon or germanium,

30 $R^{6A}-R^{11A}$ are each, independently of one another, hydrogen, C_1 - C_{20} -alkyl, C_2 - C_{20} -alkenyl, C_6 - C_{20} -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or SiR^{12A}_3 , where the organic radicals $R^{6A}-R^{11A}$ may also be substituted by halogens and two geminal or vicinal radicals $R^{6A}-R^{11A}$ may also be joined to form a five- or six-membered ring and

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R^{12A} the radicals R^{12A} are each, independently of one another, hydrogen, C_1 - C_{20} -alkyl, C_2 - C_{20} -alkenyl, C_6 - C_{20} -aryl or alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part, C_1 - C_{10} -alkoxy or C_6 - C_{10} -aryloxy and two radicals R^{12A} may also be joined to form a five- or six-membered ring, and

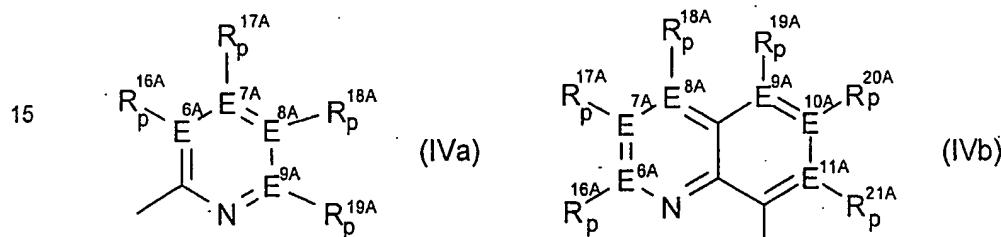
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A is an uncharged donor group containing one or more atoms of group 15 and/or 16 of the Periodic Table of the Elements or a carbene, preferably an unsubstituted, substituted or fused, heteroaromatic ring system,

5 M^A is a metal selected from the group consisting of titanium in the oxidation state 3, vanadium, chromium, molybdenum and tungsten and

k is 0 or 1.

10 4. A monocyclopentadienyl complex as claimed in any of claims 1 to 3 in which A is a group of
the formula (IVa) or (IVb):



20 where

$E^{6A}-E^{11A}$ are each, independently of one another, carbon or nitrogen.

R^{16A} - R^{21A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or SiR^{22A}₃, where the organic radicals R^{16A- R^{21A} may also be substituted by halogen(s) or nitrogen and further C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or SiR^{22A}₃ groups and two vicinal radicals R^{16A- R^{21A} or R^{16A} and Z may also be joined to form a five- or six-membered ring and}}

R^{22A} the radicals R^{22A} are each, independently of one another, hydrogen, C_1-C_{20} -alkyl, C_2-C_{20} -alkenyl, C_6-C_{20} -aryl or alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two radicals R^{22A} may also be joined to form a five- or six-membered ring and

p is 0 when $E^{6A} - E^{11A}$ is nitrogen and is 1 when $E^{6A} - E^{11A}$ is carbon.

5. A monocyclopentadienyl complex as claimed in claim 3 or 4 in which -Z-A and the aryl substituent are in the 1,3-positions relative to one another.

6. A catalyst system for olefin polymerization comprising

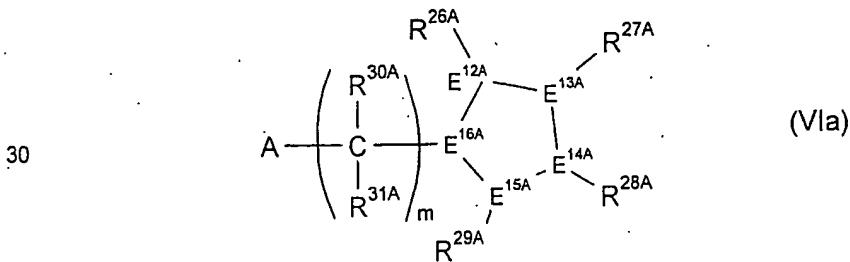
- A) at least one monocyclopentadienyl complex according to claims 1 to 5,
- 5 B) optionally an organic or inorganic support,
- C) optionally one or more activating compounds,
- 10 D) optionally further catalysts suitable for olefin polymerization and
- E) optionally one or more metal compounds containing a metal of group 1, 2 or 13 of the Periodic Table.

15 7. A prepolymerized catalyst system comprising a catalyst system as claimed in claim 6 and one or more linear C₂-C₁₀-1-alkenes polymerized onto it in a mass ratio of from 1:0.1 to 1:1 000 based on the catalyst system.

20 8. The use of a catalyst system as claimed in claim 6 or 7 for the polymerization or copolymerization of olefins.

9. A process for preparing polyolefins by polymerization or copolymerization of olefins in the presence of a catalyst system as claimed in claim 6 or 7.

25 10. A process for preparing cyclopentadiene systems of the formula (Vla),



35 where the variables have the following meanings:

E^{12A} - E^{16A} are each carbon, with four adjacent E^{12A} - E^{16A} forming a conjugated diene system and the remaining E^{12A} - E^{16A} additionally bearing a hydrogen,

R^{26A} - R^{29A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part, NR^{32A}₂, N(SiR^{32A}₃)₂, OR^{32A}, OSiR^{32A}₃, BR^{32A}₂, SiR^{32A}₃, where the organic radicals R^{26A}-R^{29A} may also be substituted by halogens and two vicinal radicals R^{26A}-R^{29A} may also be joined to form a five- or six-membered ring, and/or two vicinal radicals R^{26A}-R^{29A} are joined to form a heterocycle which contains at least one atom from the group consisting of N, P, O or S,

5 R^{30A}-R^{31A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or SiR^{32A}₃, where the organic radicals R^{30A}-R^{31A} may also be substituted by halogens and R^{30A} or R^{31A} and A may also be joined to form a five- or six-membered ring,

10 R^{32A} the radicals R^{32A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals R^{32A} may also be joined to form a five- or six-membered ring,

15 m is 0, 1 or 2,

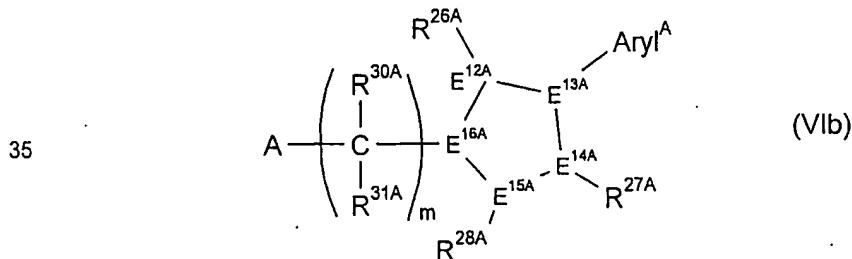
20 A is an uncharged donor group containing one or more atoms of group 15 and/or 16 of the Periodic Table of the Elements or a carbene, preferably an unsubstituted, substituted or fused, heteroaromatic ring system,

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which comprises:

a) reacting an (A-(CR^{29A}R^{30A})_m)⁻ anion with a cyclopentanedione or a silyl ether of an enolised cyclopentanedione.

30 11. A process for preparing cyclopentadiene systems of the formula (Vlb),



40 where the variables have the following meanings:

$E^{12A}-E^{16A}$ are each carbon, with four adjacent $E^{12A}-E^{16A}$ forming a conjugated diene system and the remaining $E^{12A}-E^{16A}$ additionally bearing a hydrogen,

$R^{26A}-R^{28A}$ are each, independently of one another, hydrogen, C_1-C_{20} -alkyl, C_2-C_{20} -alkenyl, C_6-C_{20} -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part, SiR^{32A}_3 , where the organic radicals $R^{26A}-R^{28A}$ may also be substituted by halogens and two vicinal radicals $R^{27A}-R^{28A}$ may also be joined to form a five- or six-membered ring, and/or two vicinal radicals $R^{27A}-R^{28A}$ are joined to form a heterocycle which contains at least one atom from the group consisting of N, P, O or S,

$R^{30A}-R^{31A}$ are each, independently of one another, hydrogen, C_1-C_{20} -alkyl, C_2-C_{20} -alkenyl, C_6-C_{20} -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or SiR^{32A}_3 , where the organic radicals $R^{30A}-R^{31A}$ may also be substituted by halogens and R^{30A} or R^{31A} and A may also be joined to form a five- or six-membered ring,

R^{32A} the radicals R^{32A} are each, independently of one another, hydrogen, C_1-C_{20} -alkyl, C_2-C_{20} -alkenyl, C_6-C_{20} -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals R^{32A} may also be joined to form a five- or six-membered ring,

Aryl^A is C_6-C_{22} -aryl, for example phenyl, naphthyl, biphenyl, anthracenyl or phenanthrenyl, which may also be substituted by N-, P-, O- or S-containing substituents, C_1-C_{22} -alkyl, C_2-C_{22} -alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms and

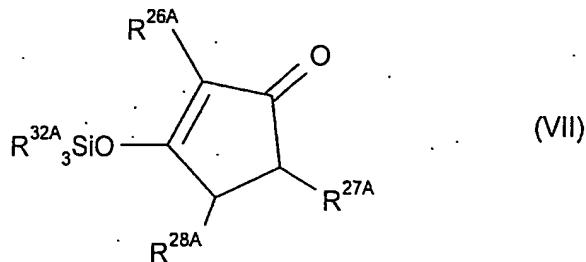
m is 0 or 1,

A is an unsubstituted, substituted or fused heteroaromatic ring system,

which comprises:

a) reacting an $(A-(CR^{30A}R^{31A})_m)^-$ anion with a cyclopentenone system of the formula (VII)

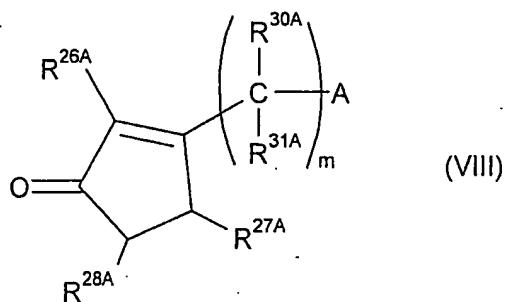
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(VII)

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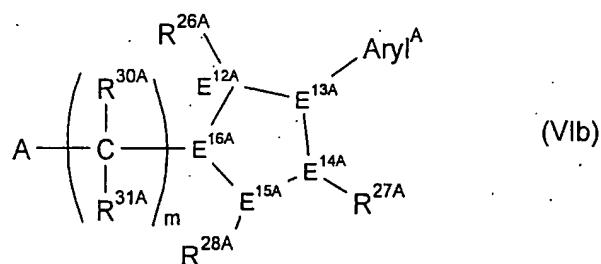
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12. A cyclopentadiene system of the formula (VIb),

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E^{12A}-E^{16A} are each carbon, with four adjacent E^{12A}-E^{16A} forming a conjugated diene system and the remaining E^{12A}-E^{16A} additionally bearing a hydrogen,

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R^{26A}-R^{28A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part, SiR^{32A}₃, where the organic radicals R^{26A}-R^{28A} may also be substituted by halogens and two vicinal radicals R^{27A}-R^{28A} may also be joined to form a five- or six-membered ring, and/or two vicinal radicals R^{27A}-R^{28A} are joined to form a heterocycle which contains at least one atom from the group consisting of N, P, O or S,

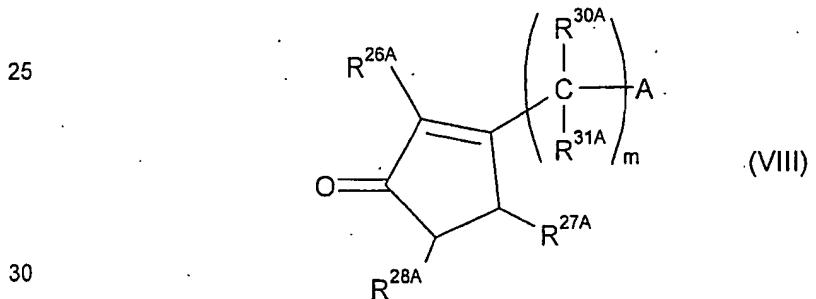
5 R^{30A} - R^{31A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or SiR^{32A}₃, where the organic radicals R^{30A}-R^{31A} may also be substituted by halogens and R^{30A} or R^{31A} and A may also be joined to form a five- or six-membered ring,

10 R^{32A} the radicals R^{32A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals R^{32A} may also be joined to form a five- or six-membered ring,

15 Aryl^A is C₆-C₂₂-aryl, for example phenyl, naphthyl, biphenyl, anthracenyl or phenanthrenyl, which may also be substituted by N-, P-, O- or S-containing substituents, C₁-C₂₂-alkyl, C₂-C₂₂-alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms and

20 m is 0 or 1 and
A is an unsubstituted, substituted or fused heteroaromatic ring system.

13. A cyclopentenone of the formula (VIII)



where the variables have the following meanings:

35 R^{26A}-R^{28A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part, SiR^{32A}₃, where the organic radicals R^{26A}-R^{28A} may also be substituted by halogens and two vicinal radicals R^{27A}-R^{28A} may also be joined to form a five- or six-membered ring, and/or two vicinal radicals R^{27A}-R^{28A} are joined to form a heterocycle which contains at least one atom from the group consisting of N, P, O or S,

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5 R^{30A} - R^{31A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or SiR^{32A}₃, where the organic radicals R^{30A}-R^{31A} may also be substituted by halogens and R^{30A} or R^{31A} and A may also be joined to form a five- or six-membered ring,

10 R^{32A} the radicals R^{32A} are each, independently of one another, hydrogen, C₁-C₂₀-alkyl, C₂-C₂₀-alkenyl, C₆-C₂₀-aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals R^{32A} may also be joined to form a five- or six-membered ring,

15 Aryl^A is C₆-C₂₂-aryl, for example phenyl, naphthyl, biphenyl, anthracenyl or phenanthrenyl, which may also be substituted by N-, P-, O- or S-containing substituents, C₁-C₂₂-alkyl, C₂-C₂₂-alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms and

20 m is 0 or 1 and
A is an unsubstituted, substituted or fused heteroaromatic ring system.

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